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A note on Sombor indices of cacti

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Abstract. The Sombor index is a novel degree based topological index, based on geometrical considerations. For a graph G, the Sombor index is defined as the sum over all edges uv of G of the terms $\sqrt{d_u^2 + d_v^2}$ where d_u, d_v denote the degrees of the end vertices of uv. In this paper, we determine the first two graphs with maximum Sombor and exponential Sombor indices among cacti of a fixed order and fixed number of cycles. We also characterize such extremal cacti for reduced Sombor index, average Sombor index and p-Sombor index, as well as for generalized Sombor index. By this we extend the results by Das [3] and Liu [13].

1. Introduction

Topological indices are graph invariants which are used to predict structural properties of chemical compounds. Among the large number of such invariants that nowadays are studied in mathematics and mathematical chemistry [11, 23], a family of vertex-degree-based topological indices were recently conceived, based on geometric considerations [8, 9]. This are the so-called Sombor index and its congeners. Of their several noteworthy applications we mention here just a few [1, 10, 14, 19, 20]. Results of their mathematical investigations are found in the review [15] and the recent papers [2, 3, 5, 6, 12, 16–18, 21, 22].

The different variants of Sombor indices can be defined in unison as follows

$$sTI(G) = \sum_{uv\in E} \phi_\alpha(f(d_u), f(d_v)) \tag{1}$$

where $\phi_\alpha(x, y) = \sqrt[\alpha]{x^\alpha + y^\alpha}$. Similarly, the generalized Sombor index can be defined as

$$gTI(G) = \sum_{uv\in E} \mu_\alpha(f(d_u), f(d_v))$$

where $\mu_\alpha(x, y) = (x^2 + y^2)^\alpha$ and d_u, d_v denote the degree of the vertices u, v respectively. The analogous

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exponential versions can be defined as,

$$esTI(G) = \sum_{uv\in E} e^{\phi_\alpha(f(d_u),f(d_v))}$$
$$egTI(G) = \sum_{uv\in E} e^{\mu_\alpha(f(d_u),f(d_v))}\,.$$

In (1) if we put $\alpha = 2$ and $f(x) = x$, the we get the ordinary Sombor index $SO(G)$, For $\alpha = 2$ and $f(x) = x-1$ we get the reduced Sombor index $SO_{red}(G)$, whereas for $\alpha = 2$ and $f(x) = x - \frac{2m}{n}$ (where n, m are order and size of the underlying graph) we get the average Sombor index $SO_{avg}(G)$. For $\alpha = p$ and $f(x) = x$, we get the p-Sombor index $SO_p(G)$. The reduced p-Sombor index and average p-Sombor index can then be constructed by taking $\alpha = p$ and $f(x) = x - 1$, and $\alpha = p$ and $f(x) = x - \frac{2m}{n}$, respectively.

Cacti's are connected graphs in which any two distinct cycles have at most one common vertex. Let $\mathcal{C}_{n,k}$ denote the collection of all cacti of order n having exactly k cycles. If all the k cycles in $G \in \mathcal{C}_{n,k}$ are triangles (i.e., C_3) then the cactus is called a triangular cactus. Cactus bundles are cactus graphs in which every cycle and trees are attached at a common vertex. The cactus bundle consisting of k triangles along with $n-2k-1$ pendent edges attached at a common vertex is called triangular cactus bundle, and is denoted by $C^0_{n,k}$. Let $C^1_{n,k}$ denote the cactus of order n having k cycles C_3 and $n - 2k - 2$ pendent edges attached at a common vertex and one pendent edge attached at a different vertex of the cycle C_3. Let $\mathcal{U}_n$ denote the collection of all unicyclic graphs of order n, and $U_{3,n-3}$ denote the unicyclic graph with a triangle C_3 along with $n - 3$ pendent edges attached at a vertex u of the cycle C_3.

For a vertex u of a graph G, let $N_G(u)$ denote the collection of all vertices of G, adjacent to the vertex u.

Several works concerning bounds and extremal graphs for the Sombor indices of cacti can be found in [7, 13, 24]. However, all these works consider different versions of the Sombor index individually. In the present work, we propose a unified method to determine the extremal cactus graphs that attain the maximum values of various versions of the Sombor and exponential Sombor indices. We also determine the second maximal value for all classes of Sombor indices for cacti. By extending this approach, we can determine higher-order extremal graphs for all classes of Sombor indices for cacti.

2. Main Results

In order to prove the main results, we first state a few auxiliary lemmas.

Lemma 2.1. *If $x \geq 1, y \geq 1, \alpha > 1$, then $\phi_\alpha(x, y) = \sqrt[\alpha]{x^\alpha + y^\alpha}$ is an increasing function with respect to x (resp. y).*

Proof.

$$\frac{\partial\phi_\alpha(x,y)}{\partial x} = x^{\alpha-1}(x^\alpha + y^\alpha)^{\frac{1}{\alpha}-1} > 0\,.$$

Since, $\phi_\alpha(x, y)$ is a symmetric function with respect to x and y, we get the result. □

Lemma 2.2. *If $x \geq 1, y \geq 1, \alpha > 1, k > 0$, then $\phi'_\alpha(x, y) = \sqrt[\alpha]{x^\alpha + y^\alpha} - \sqrt[\alpha]{x^\alpha + (y-k)^\alpha}$ is a decreasing function with respect to x.*

Proof.

$$\frac{\partial\phi'_\alpha(x,y)}{\partial x} = x^{\alpha-1}(x^\alpha + y^\alpha)^{\frac{1}{\alpha}-1} - x^{\alpha-1}(x^\alpha + (y-k)^\alpha)^{\frac{1}{\alpha}-1} < 0$$

since, $x \geq 1, y \geq 1, \alpha > 1, k > 0$. □

Lemma 2.3. *If $x \geq 1, y \geq 1, \alpha > 1, k > 0$, then $\phi'_\alpha(x, y) = \sqrt[\alpha]{x^\alpha + y^\alpha} - \sqrt[\alpha]{x^\alpha + (y-k)^\alpha}$ is an increasing function with respect to y.*

Proof.

$$\frac{\partial \phi'_\alpha(x,y)}{\partial y} = y^{\alpha-1}(x^\alpha + y^\alpha)^{\frac{1}{\alpha}-1} - (y-k)^{\alpha-1}(x^\alpha + (y-k)^\alpha)^{\frac{1}{\alpha}-1} = \left(\frac{x^\alpha}{y^\alpha}+1\right)^{\frac{1}{\alpha}-1} - \left(\frac{x^\alpha}{(y-k)^\alpha}+1\right)^{\frac{1}{\alpha}-1} > 0$$

since, $x \geq 1, y \geq 1, \alpha > 1, k > 0$. □

Lemma 2.4. *If $x \geq 1, y \geq 1, \alpha > 1$, then $\phi_\alpha(x, n-x) = \sqrt[\alpha]{x^\alpha + (n-x)^\alpha}$ is an is an increasing function with respect to x when $x \geq \frac{n}{2}$ and is a decreasing function when $x < \frac{n}{2}$.*

Proof.

$$\frac{\partial \phi_\alpha(x,(n-x))}{\partial x} = (x^{\alpha-1} - ((n-x)^{\alpha-1}))(x^\alpha + (n-x)^\alpha)^{\frac{1}{\alpha}-1}\,.$$

Then, $(x^{\alpha-1} - ((n-x)^{\alpha-1})) > 0$ when $x \geq \frac{n}{2}$ and $(x^{\alpha-1} - ((n-x)^{\alpha-1})) < 0$ when $x < \frac{n}{2}$. □

As a consequence, we have a following

Corollary 2.5.

$$\phi_\alpha(n-1,1) > \phi_\alpha(n-2,2) > \cdots > \phi_\alpha\left(\left\lceil \frac{n}{2} \right\rceil, \left\lfloor \frac{n}{2} \right\rfloor\right).$$

Lemma 2.6. *If $x \geq 1, y \geq 1, \alpha > 1$, then $\mu_\alpha(x,y) = (x^2+y^2)^\alpha$ is an increasing function with respect to x (resp. y).*

Proof.

$$\frac{\partial \mu_\alpha(x,y)}{\partial x} = 2x\alpha(x^2+y^2)^{\alpha-1} > 0\,.$$

Now, $\mu_\alpha(x,y)$ is a symmetric function with respect to x and y, we get the result. □

Lemma 2.7. *If $x \geq 1, y \geq 1, \alpha > 1$, then $\mu'_\alpha(x,y) = (x^2+y^2)^\alpha - (x^2+(y-k)^2)^\alpha$ is an increasing function with respect to x.*

Proof. By direct computation,

$$\frac{\partial \mu_\alpha(x,y)}{\partial x} = 2x\alpha(x^2+y^2)^{\alpha-1} - 2x\alpha(x^2+(y-k)^2)^{\alpha-1} > 0\,.$$

□

Lemma 2.8. *If $x \geq 1, y \geq 1, \alpha > 1$, then $\mu'_\alpha(x,y) = (x^2+y^2)^\alpha - (x^2+(y-k)^2)^\alpha$ is an increasing function with respect to y.*

Proof. By direct computation,

$$\frac{\partial \mu_\alpha(x,y)}{\partial y} = 2y\alpha(x^2+y^2)^{\alpha-1} - 2(y-k)\alpha(x^2+(y-k)^2)^{\alpha-1} > 0\,.$$

□

Lemma 2.9. *If $x \geq 1, y \geq 1, \alpha > 1$, then $\mu_\alpha(x, n-x) = (x^2+(n-x)^2)^\alpha$ is an increasing function with respect to x when $x \geq \frac{n}{2}$ and is a decreasing function when $x < \frac{n}{2}$.*

Proof.

$$\frac{\partial \mu_\alpha(x,(n-x))}{\partial x} = (4x-2n)\alpha(x^2+(n-x)^2)^{\alpha-1} > 0\,,$$

now, $(4x-2n)\alpha(x^2+(n-x)^2)^{\alpha-1} > 0$ when $x \geq \frac{n}{2}$ and $(4x-2n)\alpha(x^2+(n-x)^2)^{\alpha-1} < 0$ when $x < \frac{n}{2}$. □

As a consequence, we have a following

Corollary 2.10.

$$\mu_\alpha(n-1,1) > \mu_\alpha(n-2,2) > \cdots > \mu_\alpha\left(\left\lceil \frac{n}{2}\right\rceil, \left\lfloor \frac{n}{2}\right\rfloor\right).$$

Let $G \in \mathcal{C}_{n,k}$ be a cactus and u be a vertex in a cycle. By $T(u)$ denote the tree attached at the vertex u.

Transformation 2.11. *Let $G \in \mathcal{C}_{n,k}$ be a cactus, u a vertex belonging to a cycle, and $T(u)$ the tree attached at the vertex u, such that $|E(T(u))| = m$. Let G' be the graph obtained from G by deleting all the edges of $T(u)$ and connecting all the vertices of $T(u)$ other than u to u (i.e., attaching m pendent edges to u), see Figure 1. Then*

$$G \cong G - E(T(u)) + \{uv : v \in T(u), v \neq u\}\,.$$

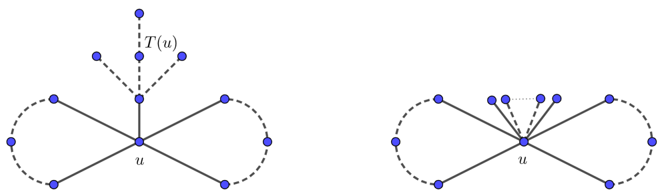

Figure 1: The graphs G and G' of Transformation 2.11

Lemma 2.12. *Let $G \in \mathcal{C}_{n,k}$ and G' be the graph obtained as in Tranfromation 2.11 where $T(u) \ncong S_{m+1}$. Then*

(a.) $sTI(G) < sTI(G')$.

(b.) $gTI(G) < gTI(G')$.

Proof. All the vertices except $x \in T(u)$ have same degree in G and G'. Let d'_u denote the degree contribution of all the edges to u other than the edges of $T(u)$. Then,

$$sTI(G) - sTI(G') = \sum_{xy \in T(u)} \phi_\alpha(d_x,d_y) + \sum_{\substack{ux \\ ux \notin T(u)}} \phi_\alpha(d_u,d_x) - \sum_{xy \in T(u)} \phi_\alpha(d'_u+m,1) - \sum_{\substack{ux \\ ux \notin T(u)}} \phi_\alpha(d'_u+m,d_x) < 0$$

since $T(u) \ncong S_{m+1}$, $d_u < d'_u + m$. Therefore, by Lemma 2.1, $\phi_\alpha(d_u,d_x) < \phi_\alpha(d'_u+m,d_x)$. Also, for every $xy \in T(u)$, $\phi_\alpha(d_x,d_y) < \phi_\alpha(d_x+d_y-1,1) < \phi_\alpha(d'_u+m,1)$ by Lemmas 2.1, 2.4, and as $d_x+d_y-1 \leq d'_u+m$. Similarly,

$$gTI(G) - gTI(G') = \sum_{xy \in T(u)} \mu_\alpha(d_x,d_y) + \sum_{\substack{ux \\ ux \notin T(u)}} \mu_\alpha(d_u,d_x) - \sum_{xy \in T(u)} \mu_\alpha(d'_u+m,1) - \sum_{\substack{ux \\ ux \notin T(u)}} \mu_\alpha(d'_u+m,d_x) < 0$$

since $T(u) \ncong S_{m+1}$, $d_u < d'_u + m$. Therefore, by Lemma 2.4, $\mu_\alpha(d_u,d_x) < \mu_\alpha(d'_u+m,d_x)$. Also, for every $xy \in T(u)$ $\mu_\alpha(d_x,d_y) < \mu_\alpha(d_x+d_y-1,1) < \mu_\alpha(d'_u+m,1)$ by Lemmas 2.4, 2.9, and as $d_x+d_y-1 \leq d'_u+m$. □

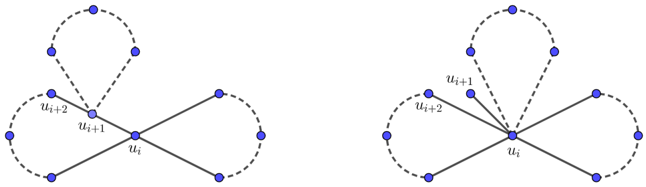

Figure 2: The graphs G and G' of Transformation 2.13

Transformation 2.13. *Let $G \in C_{n,k}$ be a cactus and $C_r = u_1u_2 \dots u_ru_1, r > 3$ be a cycle in G. Assume that $d_{u_i} \geq d_{u_{i+1}}, 1 \leq i \leq r-1$. Let G' be the graph obtained from G by deleting all the edges adjacent to u_{i+1} and adding edges connecting all the neighbors of u_{i+1} to u_i, see Figure 2. That is,*

$$G' \cong G - \bigcup_{x \in N_G(u_{i+1})} \{u_{i+1}x\} + \bigcup_{x \in N_G(u_{i+1})} \{u_ix\}.$$

Lemma 2.14. *Let $G \in C_{n,k}$ and G' be the graph obtained as in Tranfromation 2.13. Then*

(a.) $sTI(G) < sTI(G')$.

(b.) $gTI(G) < gTI(G')$.

Proof. All the vertices other than u_i, u_{i+1} have the same degree in G and G'. Therefore, all the edges other than those incident on u_i, u_{i+1} will contribute the same value to the topological index in G and G'. Therefore,

$$\begin{aligned} sTI(G) - sTI(G') = & \sum_{\substack{u_ix \\ x \neq u_{i+1}}} \phi_\alpha(d_{u_i}, d_x) + \sum_{\substack{u_{i+1}x \\ x \neq u_i}} \phi_\alpha(d_{u_i+1}, d_x) + \phi_\alpha(d_{u_i}, d_{u_{i+1}}) \\ & - \sum_{\substack{u_ix \\ x \neq u_{i+1}}} \phi_\alpha(d_{u_i} + d_{u_i+1} - 1, d_x) - \sum_{\substack{u_{i+1}x \\ x \neq u_i}} \phi_\alpha(d_{u_i} + d_{u_i+1} - 1, d_x) - \phi_\alpha(d_{u_i} + d_{u_{i+1}} - 1, 1) < 0, \end{aligned}$$

since by Lemma 2.1, for the edge u_ix, $\phi_\alpha(d_{u_i}, d_x) \leq \phi_\alpha(d_{u_i} + d_{u_i+1} - 1, d_x)$ and for the edge $u_{i+1}x$, $\phi_\alpha(d_{u_i+1}, d_x) < \phi_\alpha(d_{u_i} + d_{u_i+1} - 1, d_x)$. Also, by Corollary 2.5, $\phi_\alpha(d_{u_i}, d_{u_{i+1}}) < \phi_\alpha(d_{u_i} + d_{u_{i+1}} - 1, 1)$. Similarly,

$$\begin{aligned} gTI(G) - gTI(G') = & \sum_{\substack{u_ix \\ x \neq u_{i+1}}} \mu_\alpha(d_{u_i}, d_x) + \sum_{\substack{u_{i+1}x \\ x \neq u_i}} \mu_\alpha(d_{u_i+1}, d_x) + \mu_\alpha(d_{u_i}, d_{u_{i+1}}) \\ & - \sum_{\substack{u_ix \\ x \neq u_{i+1}}} \mu_\alpha(d_{u_i} + d_{u_i+1} - 1, d_x) - \sum_{\substack{u_{i+1}x \\ x \neq u_i}} \mu_\alpha(d_{u_i} + d_{u_i+1} - 1, d_x) - \mu_\alpha(d_{u_i} + d_{u_{i+1}} - 1, 1) < 0 \end{aligned}$$

since by Lemma 2.4, for the edge u_ix, $\mu_\alpha(d_{u_i}, d_x) < \mu_\alpha(d_{u_i} + d_{u_i+1} - 1, d_x)$ and for the edge $u_{i+1}x$, $\mu_\alpha(d_{u_i+1}, d_x) < \mu_\alpha(d_{u_i} + d_{u_i+1} - 1, d_x)$. Also, by Corollary 2.10, $\mu_\alpha(d_{u_i}, d_{u_{i+1}}) < \mu_\alpha(d_{u_i} + d_{u_{i+1}} - 1, 1)$. □

Transformation 2.15. *Let $G \in C_{n,k}$ be a triangular cacti and $C_3 = u_1u_2u_3u_1$ be a cycle in G. Assume that $d_{u_1} \geq d_{u_2} \geq d_{u_3} \geq 3$. Let G' be the graph obtained from G by deleting all the edges adjacent to u_3 other than u_1u_3, u_2u_3 and adding edges connecting all the neighbors of u_3 other than u_1, u_3 to u_1, see Figure 3. That is,*

$$G' \cong G - \bigcup_{\substack{x \in N_G(u_3) \\ x \neq u_1, x \neq u_2}} \{u_3x\} + \bigcup_{\substack{x \in N_G(u_3) \\ x \neq u_1, x \neq u_2}} \{u_1x\}.$$

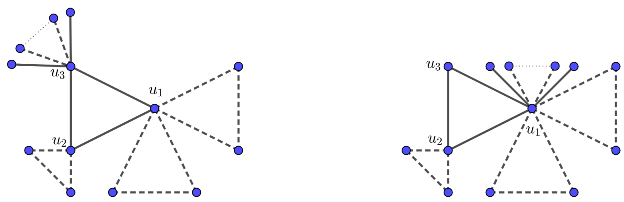

Figure 3: The graphs G and G' of Transformation 2.15.

Lemma 2.16. *Let $G \in C_{n,k}$ and G' be the graph obtained as in Transformation 2.15. Then*

(a.) $sTI(G) < sTI(G')$.

(b.) $gTI(G) < gTI(G')$.

Proof. All vertices other than u_1, u_3 have the same degree in G and G'. Therefore, all the edges other than those incident on u_1, u_3 will contribute the same value to the topological index in G and G'. Therefore,

$$\begin{aligned} sTI(G) - sTI(G') &= \sum_{\substack{u_1x \\ x\neq u_2 \\ x\neq u_3}} \phi_\alpha(d_{u_1}, d_x) + \sum_{\substack{u_3x \\ x\neq u_1 \\ x\neq u_3}} \phi_\alpha(d_{u_3}, d_x) + \phi(d_{u_1}, d_{u_2}) + \phi(d_{u_3}, d_{u_2}) + \phi_\alpha(d_{u_3}, d_{u_1}) \\ &- \sum_{\substack{u_1x \\ x\neq u_2 \\ x\neq u_3}} \phi_\alpha(d_{u_1} + d_{u_3} - 2, d_x) - \sum_{\substack{u_3x \\ x\neq u_1 \\ x\neq u_2}} \phi_\alpha(d_{u_1} + d_{u_3} - 2, d_x) \\ &- \phi_\alpha(d_{u_1} + d_{u_3} - 2, 2) - \phi_\alpha(d_{u_1} + d_{u_3} - 2, d_{u_2}) - \phi_\alpha(2, d_{u_2}) \\ &= \sum_{\substack{u_1x \\ x\neq u_2 \\ x\neq u_3}} (\phi_\alpha(d_{u_1}, d_x) - \phi_\alpha(d_{u_1} + d_{u_3} - 2, d_x)) + \sum_{\substack{u_3x \\ x\neq u_1 \\ x\neq u_3}} (\phi_\alpha(d_{u_3}, d_x) - \phi_\alpha(d_{u_1} + d_{u_3} - 2, d_x)) \\ &+ \phi'(d_{u_3}, d_{u_2}) - \phi'(d_{u_1} + d_{u_3} - 2, , d_{u_2}) + \phi_\alpha(d_{u_3}, d_{u_1}) - \phi_\alpha(d_{u_1} + d_{u_3} - 2, 2) < 0 \end{aligned}$$

since by Lemma 2.1, for the edge u_1x, $\phi_\alpha(d_{u_1}, d_x) \leq \phi_\alpha(d_{u_1} + d_{u_3} - 2, d_x)$ and for the edge u_3x, $\phi_\alpha(d_{u_3}, d_x) < \phi_\alpha(d_{u_1} + d_{u_3} - 2, d_x)$. Also, by Lemma 2.2, $\phi'(d_{u_3}, d_{u_2}) < \phi'(d_{u_1} + d_{u_3} - 2, , d_{u_2})$ as $d_{u_3} < d_{u_1} + d_{u_3} - 2$. Also by Lemma 2.1, $\phi_\alpha(d_{u_1}, d_{u_2}) < \phi_\alpha(d_{u_1} + d_{u_3} - 2, d_{u_2})$. Similarly,

$$\begin{aligned} gTI(G) - gTI(G') &= \sum_{\substack{u_1x \\ x\neq u_2 \\ x\neq u_3}} \mu_\alpha(d_{u_1}, d_x) + \sum_{\substack{u_3x \\ x\neq u_1 \\ x\neq u_3}} \mu_\alpha(d_{u_3}, d_x) + \mu_\alpha(d_{u_1}, d_{u_2}) + \mu_\alpha(d_{u_2}, d_{u_3}) + \mu_\alpha(d_{u_3}, d_{u_1}) \\ &- \sum_{\substack{u_1x \\ x\neq u_2 \\ x\neq u_3}} \mu_\alpha(d_{u_1} + d_{u_3} - 2, d_x) + \sum_{\substack{u_3x \\ x\neq u_1 \\ x\neq u_2}} \mu_\alpha(d_{u_1} + d_{u_3} - 2, d_x) \\ &- \mu_\alpha(d_{u_1} + d_{u_3} - 2, 2) - \mu_\alpha(d_{u_1} + d_{u_3} - 2, d_{u_2}) - \mu_\alpha(d_{u_2}, 2) \\ &= \sum_{\substack{u_1x \\ x\neq u_2 \\ x\neq u_3}} (\mu_\alpha(d_{u_1}, d_x) - \mu_\alpha(d_{u_1} + d_{u_3} - 2, d_x)) + \sum_{\substack{u_3x \\ x\neq u_1 \\ x\neq u_3}} (\mu_\alpha(d_{u_3}, d_x) - \mu_\alpha(d_{u_1} + d_{u_3} - 2, d_x)) \\ &+ \mu'(d_{u_3}, d_{u_2}) - \mu'(d_{u_1} + d_{u_3} - 2, , d_{u_2}) + \mu_\alpha(d_{u_3}, d_{u_1}) - \mu_\alpha(d_{u_1} + d_{u_3} - 2, 2) < 0 \end{aligned}$$

since by Lemma 2.4, for the edge u_1x, $\mu_\alpha(d_{u_1}, d_x) \leq \mu_\alpha(d_{u_1} + d_{u_3} - 2, d_x)$ and for the edge u_3x, $\mu_\alpha(d_{u_3}, d_x) < \mu_\alpha(d_{u_1} + d_{u_3} - 2, d_x)$. Also, by Lemma 2.6, $\mu'(d_{u_3}, d_{u_2}) < \mu'(d_{u_1} + d_{u_3} - 2, , d_{u_2})$ as $d_{u_3} < d_{u_1} + d_{u_3} - 2$. Also, by Lemma 2.4, $\mu_\alpha(d_{u_1}, d_{u_2}) < \mu_\alpha(d_{u_1} + d_{u_3} - 2, d_{u_2})$. □

Using these results we arrive at the following upper bounds on Sombor indices of cacti.

Theorem 2.17. *Let $G \in C_{n,k}, n \geq 8, k \geq 1$. Then*

(a.) $sTI(G) \leq (n-2k-1)(\phi(n-1,1)) + 2k(\phi(n-1,2)) + k\phi(2,2)$ *and the equality holds if and only if* $G \cong C^0_{n,k}$.

(b.) $gTI(G) \leq (n-2k-1)(\mu(n-1,1)) + 2k(\mu(n-1,2)) + k\mu(2,2)$ *and the equality holds if and only if* $G \cong C^0_{n,k}$.

Proof. Let G be the graph that attains the maximum value of the topological index among the graphs in $C_{n,k}$. Then by the repeated application of Transformation 2.11 and by Lemma 2.12, all the bridges of G must be pendent edges and by repeated application of Transformation 2.13 and by Lemma 2.14, G must be of the form of a triangular cactus whose all bridges are pendent edges. Now, by the repeated application of Transformation 2.15 and by Lemma 2.16, $G \cong C^0_{n,k}$. Then, by direct computation,

$$sTI(C^0_{n,k}) = (n-2k-1)(\phi(n-1,1)) + 2k(\phi(n-1,2)) + k\phi(2,2)$$
$$gTI(C^0_{n,k}) = (n-2k-1)(\mu(n-1,1)) + 2k(\mu(n-1,2)) + k\mu(2,2)\,.$$

□

Using the same Transformations 2.11-2.15 we can establish upper bounds of exponential Sombor index for cacti of order n having fixed number of cycles k.

Corollary 2.18. *Let $G \in C_{n,k}, n \geq 8, k \geq 1$. Then*

(a.) $esTI(G) \leq e^{((n-2k-1)(\phi(n-1,1))+2k(\phi(n-1,2))+k\phi(2,2))}$ *and the equality holds if and only if* $G \cong C^0_{n,k}$.

(b.) $egTI(G) \leq e^{((n-2k-1)(\mu(n-1,1))+2k(\mu(n-1,2))+k\mu(2,2))}$ *and the equality holds if and only if* $G \cong C^0_{n,k}$.

We now determine the cacti in $C_{n,k}$ with second greatest Sombor indices.

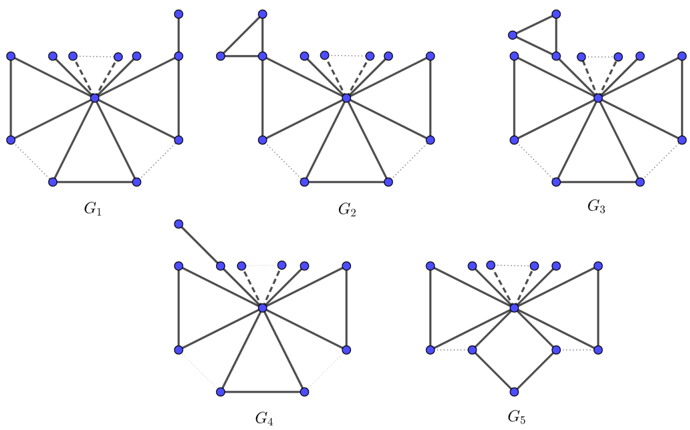

Figure 4: The graphs mentioned in Theorem 2.19.

Theorem 2.19. *Let $G \in C_{n,k} \backslash \{C^0_{n,k}\}, n \geq 12, k \geq 1$. Then*

(a.) $sTI(G) \leq (n-2k-2)\phi_\alpha(n-2,1) + (2k-1)\phi_\alpha(n-2,2) + (k-1)\phi_\alpha(2,2) + \phi_\alpha(n-2,3) + \phi_\alpha(3,1) + \phi_\alpha(3,2)$ *and the equality holds if and only if* $G \cong C^1_{n,k}$.

(b.) $gTI(G) \leq (n-2k-2)\mu_\alpha(n-2,1) + (2k-1)\mu_\alpha(n-2,2) + (k-1)\mu_\alpha(2,2) + \mu_\alpha(n-2,3) + \mu_\alpha(3,1) + \mu_\alpha(3,2)$ *and the equality holds if and only if* $G \cong C^1_{n,k}$.

Proof. Let G be the graph that attains the maximum value of topological index among graphs in $C_{n,k}\backslash\{C^0_{n,k}\}$. Then using Transformation 2.11 to Transformation 2.15 and Lemmas 2.12–Lemma 2.16, G must be a cactus bundle having the following properties.

Case I: All the pendent edges are not attached at a common vertex. Then G has exactly one pendent edge attached at a different vertex of the cycle C_3, that is, $G \cong G_1$, see Figure 4. Then by direct computation

$$\begin{aligned} sTI(G_1) =&(n-2k-2)\phi_\alpha(n-2,1) + (2k-1)\phi_\alpha(n-2,2) + (k-1)\phi_\alpha(2,2)\\ &+ \phi_\alpha(n-2,3) + \phi_\alpha(3,1) + \phi_\alpha(3,2)\,. \end{aligned}$$

Case II: All except one cycle must be an end block: Then G has one cycle C_3 which is not attached at a common vertex. Then either it must be attached at the end of a pendent vertex or some other vertex of the cycle, i.e., $G \cong G_2$ or $G \cong G_3$, see Figure 4. Then,

$$\begin{aligned} sTI(G_1) - sTI(G_2) &= (n-2k-2)\phi_\alpha(n-2,1) + (2k-1)\phi_\alpha(n-2,2) + (k-1)\phi_\alpha(2,2)\\ &+ \phi_\alpha(n-2,3) + \phi_\alpha(3,1) + \phi_\alpha(3,2) - (n-2k-1)\phi_\alpha(n-3,1)\\ &- (2k-3)\phi_\alpha(n-3,2) - (k-1)\phi_\alpha(2,2) - \phi_\alpha(n-3,4) - 3\phi_\alpha(4,2)\\ &= (n-2k-2)(\phi_\alpha(n-2,1) - \phi_\alpha(n-3,1)) + (2k-3)(\phi_\alpha(n-2,2) - \phi_\alpha(n-3,2))\\ &+ (\phi_\alpha(n-2,3) - \phi_\alpha(n-3,4)) + \phi_\alpha(n-2,2) - \phi_\alpha(n-2,1) + \phi_\alpha(n-2,2) - 2\phi_\alpha(4,2)\\ &+ \phi_\alpha(3,2) + \phi_\alpha(3,1) - \phi_\alpha(4,2) > 0 \end{aligned}$$

in view of Lemmas 2.1–Lemma 2.4 and Corollary 2.5. Also, note that $\phi_\alpha(3,2) + \phi_\alpha(3,1) > \phi_\alpha(4,2)$ and $\phi_\alpha(n-2,2) > 2\phi_\alpha(4,2)$ when $n \geq 12$. Now,

$$\begin{aligned} sTI(G_1) - sTI(G_3) &= (n-2k-2)\phi_\alpha(n-2,1) + (2k-1)\phi_\alpha(n-2,2) + (k-1)\phi_\alpha(2,2)\\ &+ \phi_\alpha(n-2,3) + \phi_\alpha(3,1) + \phi_\alpha(3,2) - (n-2k-2)\phi_\alpha(n-3,1)\\ &- (2k-2)\phi_\alpha(n-3,2) - k\phi_\alpha(2,2) - \phi_\alpha(n-3,3) - 2\phi_\alpha(3,2)\\ &= (n-2k-2)(\phi_\alpha(n-2,1) - \phi_\alpha(n-3,1)) + (2k-2)(\phi_\alpha(n-2,2) - \phi_\alpha(n-3,2))\\ &+ (\phi_\alpha(n-2,3) - \phi_\alpha(n-3,3)) + \phi_\alpha(n-2,2) + \phi_\alpha(3,2) + \phi_\alpha(3,1) - \phi_\alpha(2,2) > 0 \end{aligned}$$

by Lemma 2.2, Lemma 2.4, and Corollary 2.5.

Case III: All bridges are not pendent edges. Then G must be of the form of $G \cong G_2$ or $G \cong G_4$. Then,

$$\begin{aligned} sTI(G_1) - sTI(G_4) &= (n-2k-2)\phi_\alpha(n-2,1) + (2k-1)\phi_\alpha(n-2,2) + (k-1)\phi_\alpha(2,2)\\ &+ \phi_\alpha(n-2,3) + \phi_\alpha(3,1) + \phi_\alpha(3,2) - (n-2k-3)\phi_\alpha(n-2,1)\\ &- (2k)\phi_\alpha(n-2,2) - k\phi_\alpha(2,2) - \phi_\alpha(n-2,2) - \phi_\alpha(2,1)\\ &= \phi_\alpha(n-2,3) - \phi_\alpha(n-2,2) - (\phi_\alpha(n-2,2) - \phi_\alpha(n-2,1))\\ &+ \phi_\alpha(3,2) - \phi_\alpha(2,2) + \phi_\alpha(3,1) - \phi_\alpha(2,1) > 0 \end{aligned}$$

by Lemma 2.2, Lemma 2.3, and Corollary 2.5.

Case IV: No cycle is C_3. If G has at least one cycle which is not C_3 then it must be C_4. Thus G has the form $G \cong G_5$. Now,

$$\begin{aligned} sTI(G_1) - sTI(G_5) &= (n-2k-2)\phi_\alpha(n-2,1) + (2k-1)\phi_\alpha(n-2,2) + (k-1)\phi_\alpha(2,2)\\ &+ \phi_\alpha(n-2,3) + \phi_\alpha(3,1) + \phi_\alpha(3,2)\\ &- (n-2k-2)\phi_\alpha(n-2,1) - (2k)\phi_\alpha(n-2,2) - (k+1)\phi_\alpha(2,2)\\ &= (\phi_\alpha(n-2,3) - \phi_\alpha(n-2,2)) + \phi_\alpha(3,2) - \phi_\alpha(2,2) + \phi_\alpha(3,1) - \phi_\alpha(2,2) > 0 \end{aligned}$$

where each quantity is positive by Lemma 2.1 and Corollary 2.5. Replacing ϕ_α by μ_α and applying Lemma 2.6, Lemma 2.7, Lemma 2.9, and Corollary 2.10 we get $gTI(G_1) > gTI(G_i), i = 2,3,4,5$. Therefore, the maximum value is obtained when, $G \cong G_1 \cong C^1_{n,k}$. $\square$

As a consequence of Theorem 2.21, we have the following corollary:

Corollary 2.20. *Let $G \in C_{n,k} \backslash \{C^0_{n,k}\}, n \geq 12, k \geq 1$. Then*
(a.) $esTI(G) \leq e^{(n-2k-2)\phi_\alpha(n-2,1)+(2k-1)\phi_\alpha(n-2,2)+(k-1)\phi_\alpha(2,2)} \times e^{\phi_\alpha(n-2,3)+\phi_\alpha(3,1)+\phi_\alpha(3,2)}$
and the equality holds if and only if $G \cong C^1_{n,k}$.
(b.) $egTI(G) \leq e^{(n-2k-2)\mu_\alpha(n-2,1)+(2k-1)\mu_\alpha(n-2,2)+(k-1)\mu_\alpha(2,2)} \times e^{\mu_\alpha(n-2,3)+\mu_\alpha(3,1)+\mu_\alpha(3,2)}$
and the equality holds if and only if $G \cong C^1_{n,k}$.

As a direct consequence of Theorem 2.17, we also obtain the upper bound of these topological indices for unicyclic graphs of a given order and characterize the graph attaining the bounds by considering the particular case of $k = 1$ in $C_{n,k}$.

Theorem 2.21. *Let $G \in \mathcal{U}_n, n \geq 8$. Then*

(a.) $sTI(G) \leq (n-3)(\phi(n-1,1)) + 2(\phi(n-1,2)) + \phi(2,2)$ *and the equality holds if and only if $G \cong U_{3,n-3}$.*

(b.) $gTI(G) \leq (n-3)(\mu(n-1,1)) + 2(\mu(n-1,2)) + \mu(2,2)$ *and the equality holds if and only if $G \cong U_{3,n-3}$.*

The corresponding exponential version is:

Corollary 2.22. *Let $G \in \mathcal{U}_n, n \geq 8$. Then*

(a.) $esTI(G) \leq e^{((n-3)(\phi(n-1,1))+2(\phi(n-1,2))+\phi(2,2))}$ *and the equality holds if and only if $G \cong U_{3,n-3}$.*

(b.) $egTI(G) \leq e^{((n-3)(\mu(n-1,1))+2\mu(n-1,2))+\mu(2,2))}$ *and the equality holds if and only if $G \cong U_{3,n-3}$.*

In a similar manner, the second upper bound of Sombor indices of unicyclic graphs of a fixed order can be directly obtained using Theorem 2.19. This results in the graph $U'_{3,n-3}$, which is the graph consisting of the cycle C_3 along with $n-4$ pendent edges attached at a vertex, and one pendent edge attached at a different vertex of C_3.

3. Applications

Several different versions of the Sombor index can be expressed via the symmetric function $\phi_\alpha(x, y)$ as

$$SO(G) = \sum_{uv \in E} \phi_\alpha(f(d_u), f(d_v)).$$

Now, taking the respective values in Theorem 2.17, we straightforwardly get the following results:

Corollary 3.1. *Let $G \in C_{n,k}$, $n \geq 8, k \geq 1$, then*

(a.) $SO(G) \leq (n-2k-1)(\sqrt{(n-1)^2+1}) + 2k((\sqrt{(n-1)^2+4})) + 2\sqrt{2}k$ *and the equality holds if and only if $G \cong C^0_{n,k}$.*

(b.) $SO_{red}(G) \leq (n-2k-1)(n-2) + 2k((\sqrt{(n-2)^2+1})) + \sqrt{2}k$ *and the equality holds if and only if $G \cong C^0_{n,k}$.*

(c.) $SO_{avg}(G) \leq (n-2k-1)((\sqrt{(n-1-\frac{2(n+k-1)}{n})^2 + (1-\frac{2(n+k-1)}{n})^2}))$ $+2k((\sqrt{(n-1-\frac{2(n+k-1)}{n})^2 + (2-\frac{2(n+k-1)}{n})^2})) + k\sqrt{2}(2-\frac{2(n+k-1)}{n})$ *and the equality holds if and only if $G \cong C^0_{n,k}$.*

(d.) $SO_p(G) \leq (n-2k-1)(\sqrt[p]{(n-1)^p+1}) + 2k((\sqrt[p]{(n-1)^p+2^p})) + 2k\sqrt[p]{2}$ *and the equality holds if and only if $G \cong C^0_{n,k}$.*

Similarly, the upper bounds on the exponential Sombor indices are as follows:

Corollary 3.2. *Let $G \in C_{n,k}$, then*

(a.) $eSO(G) \leq e^{((n-2k-1)(\sqrt{(n-1)^2+1})+2k((\sqrt{(n-1)^2+4}))+2\sqrt{2}k)}$ *and the equality holds if and only if* $G \cong C^0_{n,k}$.

(b.) $eSO_{red}(G) \leq e^{((n-2k-1)(n-2)+2k((\sqrt{(n-2)^2+1}))+\sqrt{2}k)}$ *and the equality holds if and only if* $G \cong C^0_{n,k}$.

(c.) $eSO_{avg}(G) \leq e^{(n-2k-1)((\sqrt{(n-\frac{2(n+k-1)}{n})^2+(1-\frac{2(n+k-1)}{n})^2}))}$
$\times e^{(2k((\sqrt{(n-1-\frac{2(n+k-1)}{n})^2+(2-\frac{2(n+k-1)}{n})^2}))+k\sqrt{2}(2-\frac{2(n+k-1)}{n}))}$ *and the equality holds if and only if* $G \cong C^0_{n,k}$.

(d.) $eSO_p(G) \leq e^{(n-2k-1)(\sqrt[p]{(n-1)^p+1})+2k((\sqrt[p]{(n-1)^p+2^p}))+2\sqrt[p]{2}k}$ *and the equality holds if and only if* $G \cong C^0_{n,k}$.

The analogous result for the generalized Sombor index is:

Corollary 3.3. *Let $G \in C_{n,k}$, then*

$$gSO(G) \leq (n-2k-1)((n-1)^2+1)^\alpha + 2k((n-1)^2+4)^\alpha + k(8)^\alpha$$

and the equality holds if and only if $G \cong C^0_{n,k}$.

Using Theorem 2.19, we get the characterizations of the second-maximal indices.

Corollary 3.4. *Let $G \in C_{n,k} \backslash \{C^0_{n,k}\}, n \geq 8, k \geq 1$, then*

(a.) $SO(G) \leq (n-2k-2)(\sqrt{(n-2)^2+1}) + (2k-1)((\sqrt{(n-2)^2+4})) + (k-1)2\sqrt{2} + (\sqrt{(n-2)^2+9}) + \sqrt{10} + \sqrt{13}$ *and the equality holds if and only if* $G \cong C^1_{n,k}$.

(b.) $SO_{red}(G) \leq (n-2k-2)(n-3) + (2k-1)((\sqrt{(n-3)^2+1})) + (k-1)\sqrt{2} + \sqrt{(n-3)^2+4} + 2 + \sqrt{5}$ *and the equality holds if and only if* $G \cong C^1_{n,k}$.

(c.)

$$\begin{aligned}
SO_{avg}(G) \leq\; & (n-2k-2)((\sqrt{(n-2-\frac{2(n+k-1)}{n})^2+(1-\frac{2(n+k-1)}{n})^2})) \\
& + (2k-1)((\sqrt{(n-2-\frac{2(n+k-1)}{n})^2+(2-\frac{2(n+k-1)}{n})^2})) \\
& + (k-1)\sqrt{2}(2-\frac{2(n+k-1)}{n}) \\
& + (\sqrt{(n-2-\frac{2(n+k-1)}{n})^2+(3-\frac{2(n+k-1)}{n})^2}) \\
& + (\sqrt{(3-\frac{2(n+k-1)}{n})^2+(1-\frac{2(n+k-1)}{n})^2}) \\
& + (\sqrt{(3-\frac{2(n+k-1)}{n})^2+(2-\frac{2(n+k-1)}{n})^2})
\end{aligned}$$

and the equality holds if and only if $G \cong C^1_{n,k}$.

(d.) $SO_p(G) \leq (n-2k-2)(\sqrt[p]{(n-2)^p+1}) + (2k-1)((\sqrt[p]{(n-2)^p+2^p})) + (k-1)\sqrt[p]{2\times 2^p} + ((\sqrt[p]{(n-2)^p+3^p})) + ((\sqrt[p]{3^p+2^p})) + ((\sqrt[p]{3^p+1^p}))$ *and the equality holds if and only if* $G \cong C^1_{n,k}$.

The analogous bounds for the exponential Sombor indices can also be found by applying Theorem 2.19, in which case the second-maximal cactus is also $C^1_{n,k}$.

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